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Synthesis, Characterization, Anticorrosion Inhibition And Thermodynamic Studies On Co(II) And Fe(II) Mixed Ligand – Chelates

F. Alarbi [1]*, M. El-ajaily[2], M. Farhat[3] and T. Abdullah[3]

[1]*Department of Chemistry, Faculty of Education, University of fezzan, Libya*
[2]*Department of Chemistry, Faculty of Science, University of Benghazi, Benghazi, Libya*
[3]*Department of Materials and Corrosion Engineering, Faculty of Engineering, Sebha University ,Libya*

Corresponding email. *falarbi703@gmail.com*

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A B S T R A C T

This work elucidates the synthesis and structural characteristics of metal chelates derived from 2-aminothiophenol and thiourea. The chelates, formed through the condensation of thiophenol and thiourea with M(II) ions (where M = Co(II) and Fe(II)), exhibit enhanced solubility in DMF and DMSO. The chelation involves the amine nitrogen atom, phenolic oxygen atom, and thiol sulfur atom as binding sites. Identification of the prepared chelates was accomplished through XRDF analysis, as well as IR and UV-vis spectroscopy. Additionally, these chelates were explored for their corrosion inhibition properties in 0.5 M HCl and a 10% (by volume) DMF solution. The corrosion studies were conducted at varying temperatures (303 and 313K), and the associated thermodynamic parameters (ΔG, ΔH, and ΔS) were derived and discussed. Importantly, the inhibition efficiencies of the Co and Fe chelates were systematically evaluated, and the results obtained from diverse measurements exhibited excellent consistency. This comprehensive study not only contributes to the understanding of the synthesized chelates but also highlights their potential as effective corrosion inhibitors.

Introduction

Mixed-ligand complexes play integral roles in diverse biological processes, with significant applications spanning analytical and various branches of chemistry [1]. Thiols (R-SH), a group of compounds rich in (– SH) moieties, exhibit high reactivity and often form conjugates with both organic and inorganic molecules [2]. The thiol (-SH) groups, particularly those present in proteins, are crucial plasma antioxidants in vivo. Predominantly located on albumin, these thiol groups serve as major reducing agents in bodily fluids [3]. Calculating the thiol status in the body is made accessible by determining serum thiol levels [4]. Notably, aromatic thiols, such as thiophenols, display higher toxicity compared to aliphatic thiols [5]. The inhibition efficiencies of organic molecules depend on the adsorption abilities in addition to structural, mechanical, and chemical properties of the adsorption layer produced under a particular solution [6]. Generally, an effective organic corrosion inhibitor has sulfur, oxygen, and/or nitrogen atoms in the molecular structure and a hydrophobic moiety that will block the mild steel surface against the corrosive environment. However, the polar moieties in the organic inhibitor molecules are considered to be responsible for forming the adsorption film [7]. In general, the inhibition performance [8] increases in the order oxygen < nitrogen < sulfur due to their increasing propensity to make coordination bonds. Inhibitor molecules with many heteroatoms demonstrate the best corrosion inhibition in comparison to those that only have one of heteroatom. Among such corrosion inhibitors, thiosemicarbazides, especially Schiff bases, are reported as active inhibitors for various alloy−environment systems such as MS, [9] aluminum, [10] copper, [11], and zinc [12] in various corrosive environments. Schiff bases have a privileged position in the field of corrosion inhibition because they are environmentally friendly and can be easily manufactured from low-cost raw materials [13]. A new ligand (E)-2-((2-chloro-6-methylquinoline-3-yl)methylene)-N'-((E)-(2-chloro-6-methylquinoline-3-yl)methylene)hydrazine-1--*carbothiohydrazide (QH) was prepared by reacting hydrazine hydrate with carbon disulfide

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to yield thiocarbohydrazide. The thiocarbohydrazide in the second step was treated with a quinoline derivative 2-chloro-6-methylquinoline-3-carbaldehyde to yield the ligand. The ligand was identified by spectroscopic techniques FTIR, ^{1}H-NMR, and ^{13}C-NMR. Next, vanadium (V), cobalt (Co), and copper (Cu) complexes were prepared in the [M:L] ratio of 1:1. The complexes were characterized using FTIR, ESI, magnetic susceptibility, and molar conductivity. The thermal analysis (TGA) of V(IV), Co(II), and Cu(II) complexes were studied. The activation thermodynamic parameters, such as the energy of activation, enthalpy, entropy, and free energy change of the complexes, were evaluated, and the stabilities of the thermal decomposition of the complexes were discussed. [14] Four new Co(II), Ni(II), Cu(II) and Fe(III) chelates with synthesized azo Schiff base ligand (ASB) derived from Schiff base [salicylaldehyde and 2-aminothiophenol] with aniline were synthesized and characterized on the basis of various physicochemical methods including; CHNS elemental analyses, molar conductivity, magnetic moment measurements, infrared, electronic, mass and proton nuclear magnetic resonance spectra. The used techniques showed the formation of 1:1[M:L] ratio and confirm the geometrical structures of the azo Schiff base and its chelates. A square planar geometry was established for Ni(II) and Cu(II) chelates and octahedral structure for Co(II) and Fe(III) chelates. The corrosion inhibition of mild steel in 0.5M HCl using azo Schiff base as inhibitor has been studied at 30 0C. High inhibition efficiency (> 90 %) of azo Schiff base for acidic corrosion of steel was determined at its low concentration (3×10-4 M) by weight loss measurements.[15] The effect of an Carbazodithoate inhibitor on the corrosion of low carbon steel (mild steels) in 2.0 M Sulphuric acid (H_2SO_4) solution by weight loss measurements and over the temperature range 30 - 50 °C. The effects of organic compound inhibitor concentration on the corrosion rate of low carbon steel have been found to increase with inhibitor concentration ($7.5x10^{-4}$ - $4.0x10^{-3}$) M at both temperature 30 °C and 50 °C. The results were fit to all used adsorption isotherms including; Langmuir isotherm and Temkin isotherm, while a slight improvement was observed when using an organic inhibitor at temperature of 50 °C. The standard free energies of adsorption ΔGads are calculated. The inhibition efficiencies of "Methyl Carbazodithoate" obtained from the all-various measurements were in good agreement.[16] Conductometry proves particularly valuable in investigating the solvent's effect on the stability constant of complex formation in pure and mixed solvent solutions, along with its impact on thermodynamic parameters like enthalpy, entropy, and free energy in complexation processes. Moreover, conductometry provides insights into the stoichiometry of complexation reactions between various ligands and metal cations.

Materials and Methods

All chemicals used in this study are pure of BDH/Aldrich, including; thioure, 2-amino-thio phenol, ethanol, DMSO, DMF, $FeCl_2.2H_2O$, $CoCl_2.6H_2O$ and distilled water. The synthesized chelates were subjected to infrared spectra were obtained by KBr disc technique by using IFS-25DPUSR\IR spectrometer (Bruker) in the range of 400-4000 cm^{-1}). electronic spectra of the chelate were measured in DOMSO solvent using a Perkin–Elmer-Lambda β–spectrophotometer. The mass spectra were carried out by using Shimadzu QP-2010 Plus. The mass percentage of the chelates were measured in X-ray Fluorescence XRF Spectrometers CMD 650 at Chemistry Department, Sebha University, Sebha, Libya.

Synthesis of Chelates.

The chelates under investigation were synthesized by dissolving 0.01 mole;0.76 g of thioure with 0.01mole of the salts [2.85 and 2.37 gm] of, $FeCl_2.6H_2O$ and $CoCl_2.6H_2O$ respectively, in 50 ml ethanol were refluxed for one hour, then addition 0.01 mole; 1.25 g of 2-aminothiophenol with 50 mL ethanol. The obtained mixture then refluxed with stirring for 3-4 hrs. The precipitate was collected by filtration through Buchner funnel, washed several times with hot ethanol until the color of the filtrate becomes clear. The product was dried at room temperature in desiccator over anhydrous calcium chloride.

RESULTS AND DISCUSSION

The chelates are air-stable, non-hygroscopic, colored solids, insoluble in water, ethanol and methanol, partially soluble and soluble in chloroform, DMSO and DMF. The XRDF analysis data of the chelates (given in Table 1) are consistent with the calculated results from the empirical formula of each compound. The results of mass percentage measurements (Table 1) suggest that all chelates are octahedral gravimetric.[17]

Table-1: XRDF analyses and some physical properties of the chelates

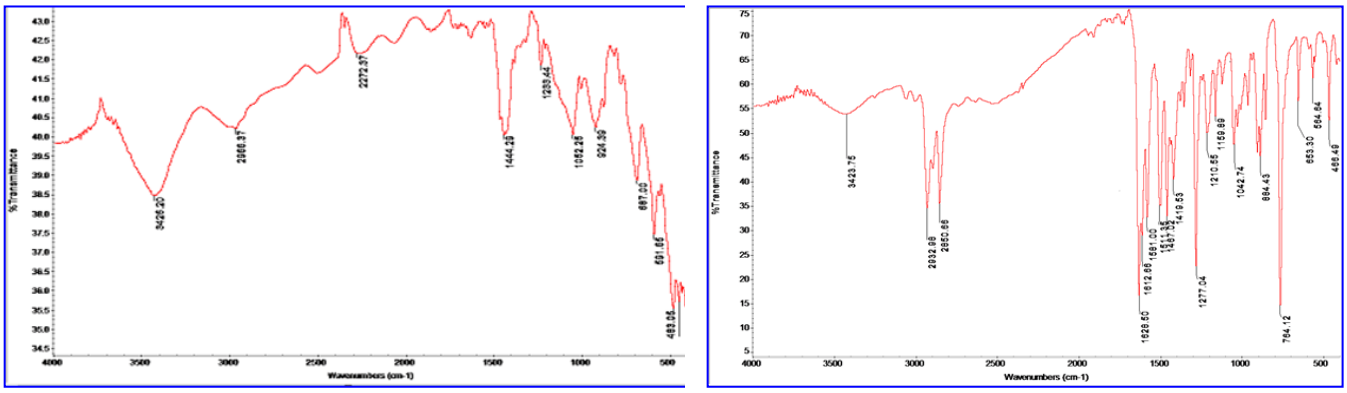
Chelates	Color	M.W	M.P °C	Mass%				Purity
				Co%	Fe %	Cl%	S%	
[Fe (L1)(L2)(Cl)$_2$]. 2H$_2$O	Light brown (sandy)	346.69	.00>360	-	62.3	0.697	25.3	72.86%
[Co(L1)(L2)(Cl)$_2$].2H$_2$O	Blackish blue	335.75	.00>360	39.9	-	15.0	29.4	87.31%

Electronic spectra of the chelates

As shown in Appendices 5 and 6, electronic spectra of chelates displayed one, two d-d transition bands of low energy in 310 (32250) cm^{-1} region and two bands of high energy in 250 (4000) cm^{-1} range as summarized in Table (2) below. The low energy bands attributed to ^2A_1g, ^2B_2g and 2Eg transitions from $2B_1g$ ground state of square planar geometry as revealed by magnetic data; broad peak structure of $2B_1g \rightarrow 2B_2g$ electronic transition band peak could be due to its mixing either with closely spaced peak of $2B_1g \rightarrow 2A_1g$ or $2B_1g \rightarrow 2Eg$ transition. The high energy peaks are assigned to metal to ligand or vice versa charge transfers. For the, Fe-complex ultraviolet spectral results show two bands at 287 nm (34843 cm^{-1}) and 350 nm (2857cm^{-1}) due to the existence of charge transfer and $^5T_2g \rightarrow ^5Eg$ transition. The obtained formation confirms an octahedral geometry for Fe(II) chelate. [18]

Infrared spectra of chelates:

The infrared spectra of the chelates of the formula Fe and Co chelates represented in figure. (1), while, the main bands and their tentative assignments are listed in table (2). The IR spectra of the chelates display broad bands in the range of 3426-3411 cm^{-1} which are attributed to the existence of water molecules .[19] Meanwhile, the same spectra show bands in range of 2966-2920 cm^{-1} attributed to υ-SH vibration, the confirmed the participation of this group in chelation through sulfur atom .[20] The spectra of the chelates exhibit the position of the amin group υ(-NH) indicating its involvement in complexation through nitrogen atom .[21] Also the same spectra exhibit bands in the range of 887-760 cm^{-1} , 691-612 cm^{-1} and 483-441 cm^{-1} which are not present in the complexes are assigned to υ(M-O) , υ(M-Cl) and υ(M-N) vibrations , and the appearance of these vibrations support the involvement of oxygen , chlorine and nitrogen atoms of the OH and NH groups in chelation process.



(**a**) (**b**)

Figure 1. (a) IR spectrum of the Co - chelate.; (b) IR spectrum of the Fe - chelate.

Table 2: Infrared and electronic spectral data of the chelates

	IR Bands (cm^{-1})								nm (cm^{-1})	
chelates	**νOH (H_2O)**	**νSH**		**υ-NH**	**ν`M-S**	**νM-O**	**νC=S**	**νM-N**	**n- π*** nm(cm^{-1})	**π- π*** nm(cm^{-1})
[Fe (L1)(L2)$(Cl)_2$]. ($2H_2O$	3423	2932	2850	764	466		1277	653	350 (**2857**(	287 (**34843**)
[Co(L1)(L2)$(Cl)_2$].$2H_2$ O	3426	2966	2272	887	483		1052	691	310 (**32250**)	250 (**4000**)

Chemical composition of Medium Carbon Steel:

The Medium steel test sample that was used for the experiment were found from steel market in Sebha had a compositional specification (in wt %) as follows 95.0% Fe, 0.45C ,1.30% Si, 0.911% Mn, 0.111% P, 0.256% S, 0.334% Cr, 0.0202% Ni, 0.491% Cu, and 0.641% Al as determined by the chemical analysis.

Corrosion Rate (CR)

The data for weight loss and corrosion rate calculations for the steel samples using chelate's are given table (4), From the obtained results, we noticed through the curve of figure (3) (4) we note that the corrosion rate decreases

as the inhibitor concentration increases and decreases significantly with an increase in temperature, the reason for the decrease is due to the increased accumulation of adsorbed inhibitor molecules on the surface of metal and the formation of a protective film against acid corrosion attack.

Table 4: corrosion rate calculations for the steel samples using Fe and Co Chelate's

	Fe- chelate			**Co-** chelate		
S. No.	Inhibitor concentration in 0.5 M HCl × 10^{-3}	CR (mg)/cm^2. min*10^{-3}, 30 °C	CR (mg)/cm^2. min*10^{-3}, 40 °C	Inhibitor concentration in 0.5 M HCl× 10^{-3}	CR (mg)/cm^2. min*10^{-3}, 30 °C	CR (mg)/cm^2. min*10^{-3}, 40 °C
1	13	3.998	1.608	14	7.858	4.838
2	0.025	3.492	1.475	0.03	7.641	4.439
3	0.12	2.150	1.376	0.14	5.027	3.554
4	0.25	1.392	0.785	0.3	2.828	2.795
5	1.27	0.026	0.116	1.44	1.886	1.194

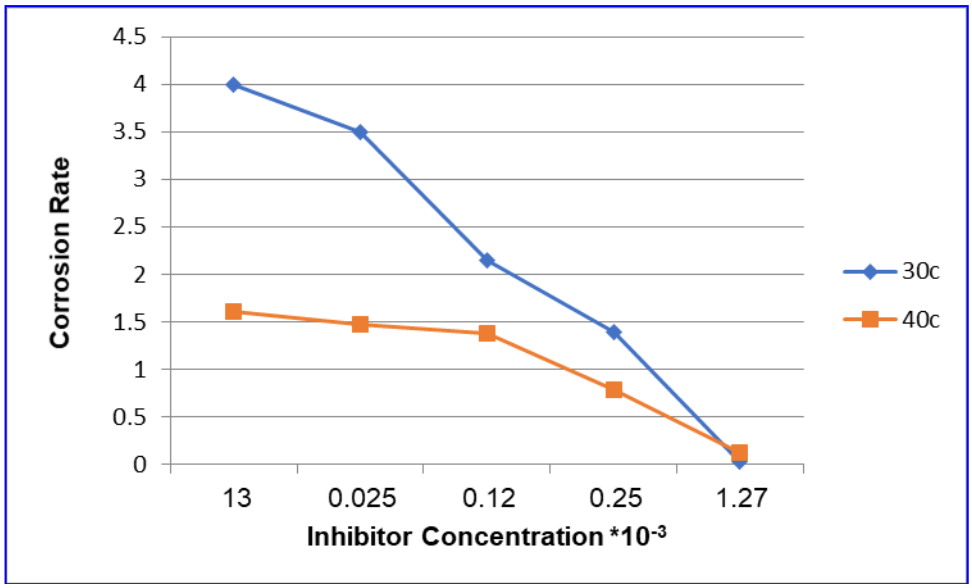


Figure (3) The Relationship between Corrosion Rate and Inhibitor Concentration at30 ˚and 40 ˚C

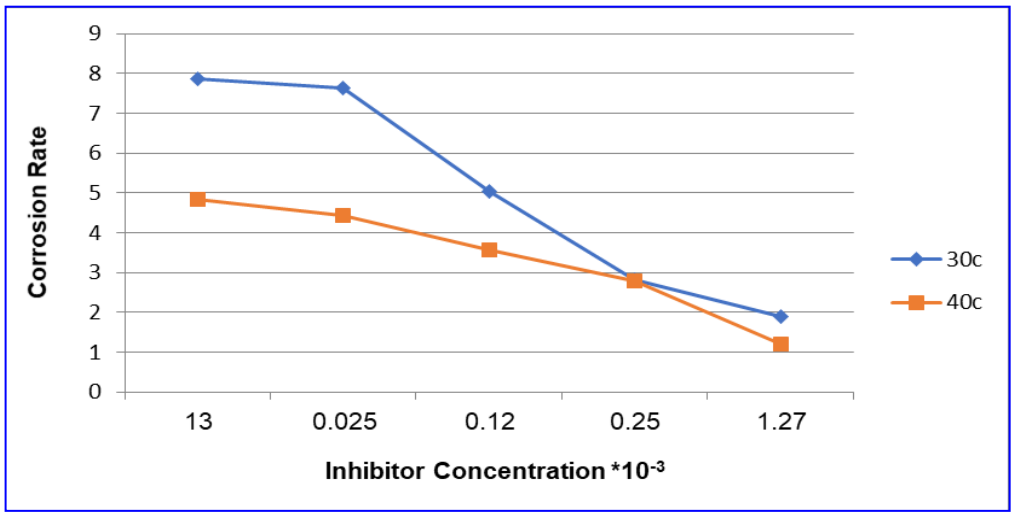


Figure (4) The Relationship between Corrosion Rate and Inhibitor Concentration at30˚ and 40˚C

Inhibition Efficiency:
The effect of inhibitor concentration on corrosion of mild carbon steel was determined using weight loss method which was out at temperature 30 and 40°C, Figure (5) (6) shows variation inhibition efficiency with different concentration, from the graph (5) (6), it can be inferred that gradual increase in inhibitor concentration increases the percentage Inhibition efficiency, hence when the inhibitor concentration increases, the corrosion rate decreases which directly increases the inhibition efficiency, of the studies showed that percentage of inhibition efficiency increases as the inhibition concentration increases.[22-23]

Table 6: inhibitory efficiency of the (Fe- Chelate) at temperatures of 30° and 40 °C.

Sample No.	Log (I)	IE % at 30 °C	IE % at 40 °C
1	0.00	0.00	0.00
2	- 4.602059991	8.32	12.65
3	-3.920818754	32.92	46.20
4	-3.602059991	52.25	65.16
5	-2.896196279	60.84	82.42

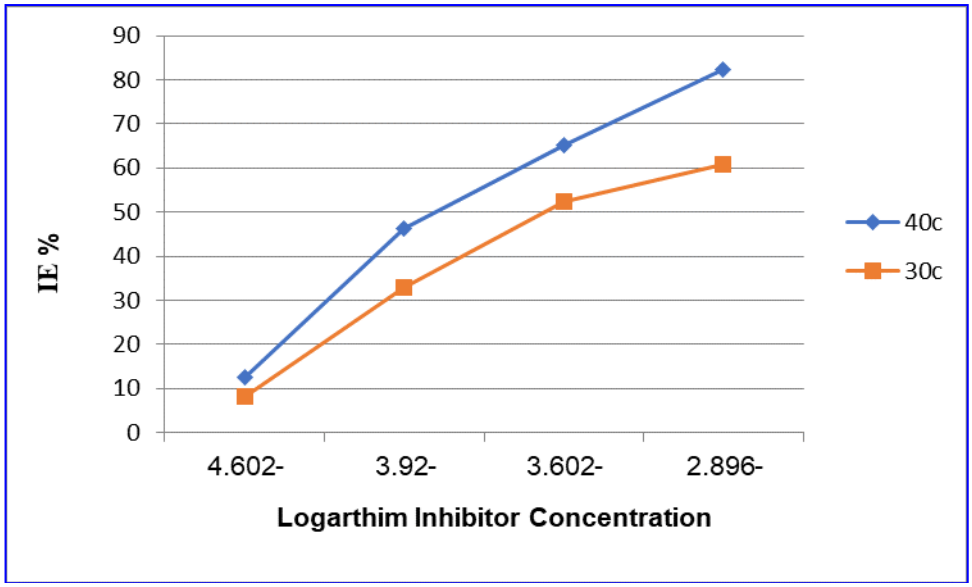


Figure (5) The Variation Inhibition Percentage with the Logarithm of the Concentration of " Fe- Chelate " HCl Containing Inhibitor Chelate, 30 and 40°C

Table 7: inhibitory efficiency of the (Co-Chelate) at temperatures of 30 and 40 °C.

Sample No.	Log (I)	IE % at 30 °C	IE % at 40 °C
1	0.00	0.00	0.00
2	- 4.540607512	22.76	26.34
3	-3.841637508	26.53	36.02
4	-3.540607512	42.23	64.01
5	-2.841637508	85.13	90.72

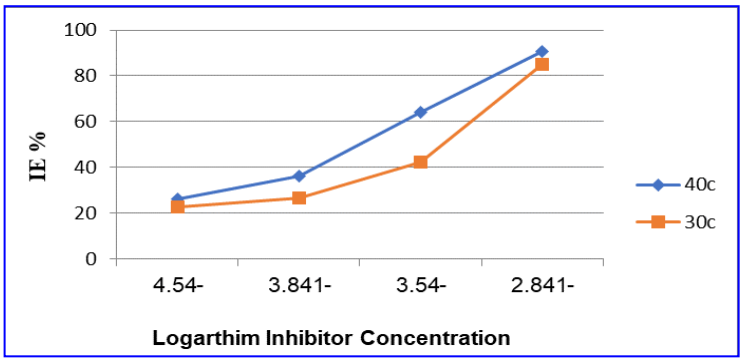


Figure (6) The Variation Inhibition Percentage with the Logarithm of the Concentration of " Co- Chelate " HCl Containing Inhibitor Chelate, 30 and 40°C

Adsorption Isotherm

Adsorption of the inhibitor molecules essentially depends on electronic characteristics of the metal surface, temperature adsorption of the solvent ionic species, the charge and the nature of the Metal surface and the electrochemical potential at the solution interface. The adsorption isotherms define the molecular interactions of the inhibitor molecules with the active sites on the metal surface. [24-26]

Two different adsorption isotherms were tested so as to have an understanding on the interface between the inhibitor and carbon steel surface. The isotherms tested were Langmuir, Temkin, the linear regression coefficient of determination (R2) was used to determine the model that fitted best to the experimental values.

Langmuir Adsorption Isotherm

Table (8)(9) provides estimated inhibitor surface coverage and adsorption energy at temperatures 30 and 40 °C. A correlation between coverage (θ) defined by (IE %) and the concentration of inhibitor (I) in electrolyte can be represented by the Langmuir adsorption isotherm.[27]

$$\theta / (1 - \theta) = K.[I] \qquad (1)$$

The obtained results are shown in table (8)(9) That the inhibitor follows isotherms of the Langmuir R is high at all temperatures, the Langmuir model assumes that the particles of This is due to the tendency 2 The inhibitor adsorbs in a dense monomolecular layer on the metal surface [28].

The value the value of adsorption constant " K " at each inhibitor concentration were calculated for two temperatures as shown on tables (8) and (9), The obtained values of adsorption constant were used to determine the Gibb's free adsorption energy ($\Delta G\ ads$) using the following equation [29].

$$K=1/55.5\ e^{(-\Delta G_{ads}/RT)} \qquad (2)$$

Adsorption process on a surface in general, negative values of Gibbs energy indicate ads in ΔG. Metallurgy takes place automatically and when the Gibbs energy values the charged metal is known as physical adsorption. [30, 31] Langmuir adsorption isotherm was found to be best fit among these four adsorption isotherms, a straight line with (R2 = 0.9606) as shown in figure (7).

Table 8: Estimated Inhibitor Surface Overage and Adsorption Energy at Temperature of 30 °C and 40 °C (Fe- Chelate)

	Fe- Chelate at 30°C			Fe- Chelate at 40°C		
S. No.	**Surface Overage (θ)**	**Adsorption constant (K) M^{-1}**	**Adsorption Energy (ΔG_{ads}) KJ/mol**	**Surface Overage (θ)**	**Adsorption constant (K) M^{-1}**	**Adsorption Energy (ΔG_{ads}) KJ/mol**
1	0.00	0.00	0.00	0.00	0.00	0.00
2	0.1265	144.84	-22.40	0.0832	90.76	-28.31

3	0.4620	171.78	-22.82	0.3293	98.19	-28.57
4	0.6516	171.04	-23.03	0.5226	109.46	-28.94
5	0.8242	195.80	-21.32	0.6063	131.97	-29.56

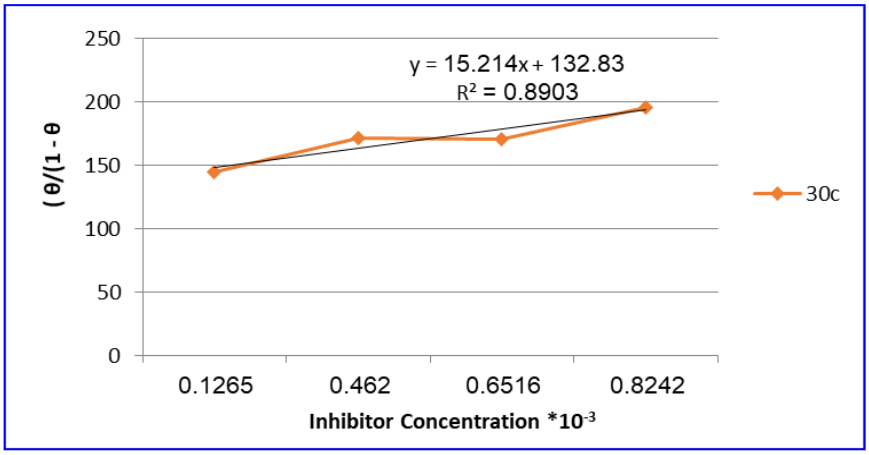


Figure (7): Langmuir Adsorption Isotherm of " Fe- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 30 ℃.

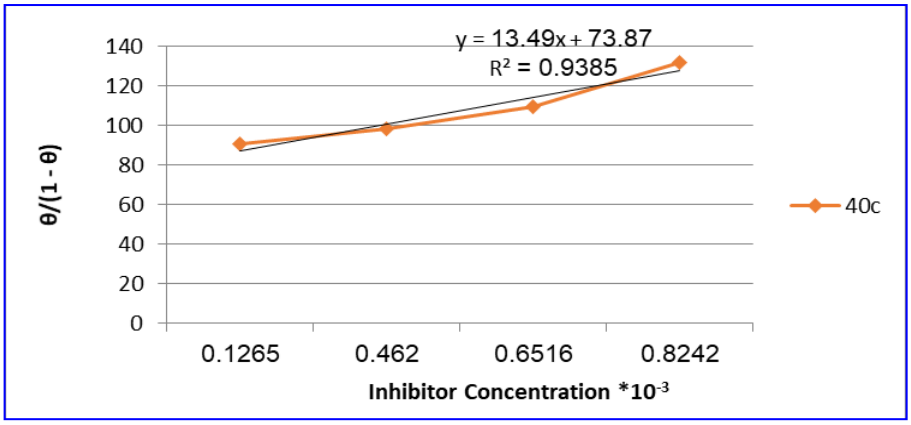


Figure (8) : Langmuir Adsorption Isotherm of " Fe- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 40 ℃.

Table 9: Estimated Inhibitor Surface Overage and Adsorption Energy at Temperature of 30 ℃ at 40℃ "Co- Chelate"

	Co- Chelate at 30 °C			Co- Chelate at 40°C		
S.No.	**Surface Overage (θ)**	**Adsorption constant (K) M^{-1}**	**Adsorption Energy (ΔG_{ads}) KJ/ mol**	**Surface Overage (θ)**	**Adsorp-tion con-stant (K) M^{-1}**	**Adsorption Energy (ΔG_{ads}) KJ/mol**
1	0.00	0.00	0.00	0.00	0.00	0.00
2	0.0633	67.69	-24.46	0.0276	28.43	-21.81

3	0.3602	112.60	-29.03	0.2653	72.25	-20.67
4	0.6401	177.90	-30.55	0.4223	73.12	-20.69
5	0.9078	195.71	-30.87	0.8513	114.51	-24.82

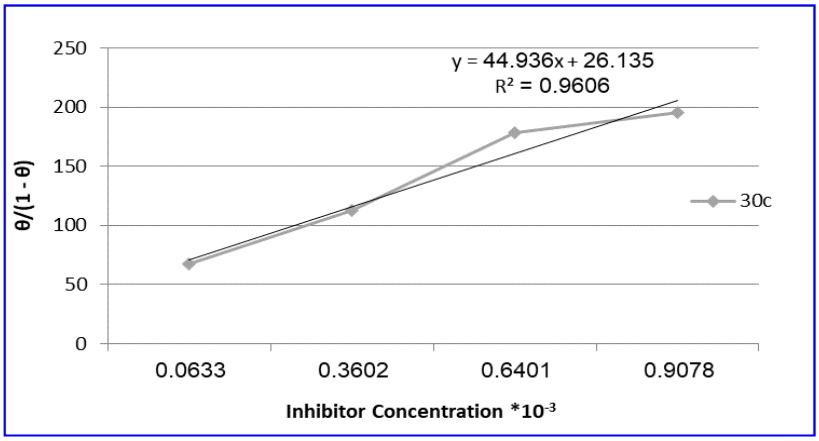


Figure (9): Langmuir Adsorption Isotherm of " Co- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 30 ℃.

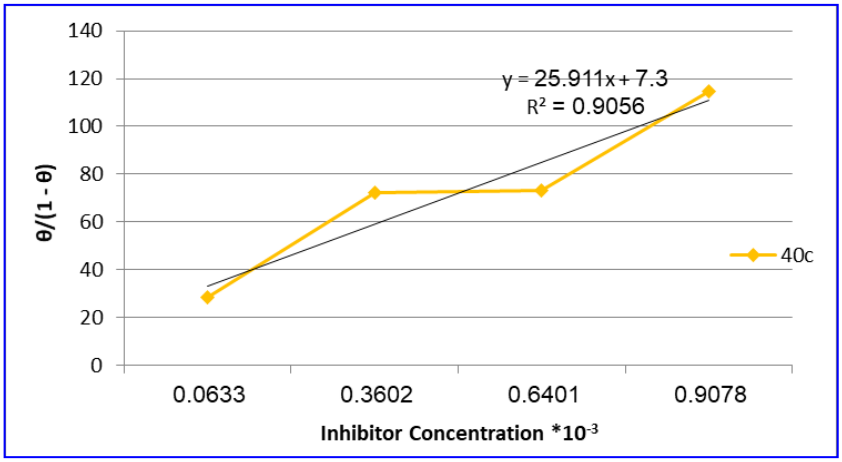


Figure (10): Langmuir Adsorption Isotherm of " Co- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 40 ℃.

Temkin Adsorption Isotherm:

This isotherm models adsorption at moderate/intermediate concentration range, assumes that adsorption heat is a function of temperature and decreases linearly as surface coverage of molecules increase [32] This is expressed in equation:

$$\mathbf{Exp\ (-2a\ \Theta) = K.\ C} \qquad \mathbf{(2)}$$

K is the equilibrium constant of the inhibitor adsorption process, a is the parameter of interaction between inhibitor molecules adsorbed on the steel surface, and θ is the degree of surface coverage, C is the inhibitor concentration.

in figures (11) (12) (13) (14) the Temkin isotherm was represented by a linear plot "Θ" versus the logarithm of inhibitor concentration "log I ".

the obtained values of the correlation "R2" for inhibitor temperatures 30 and 40 Fe- Chelate were (0.8903) and (0.9385) respectively.

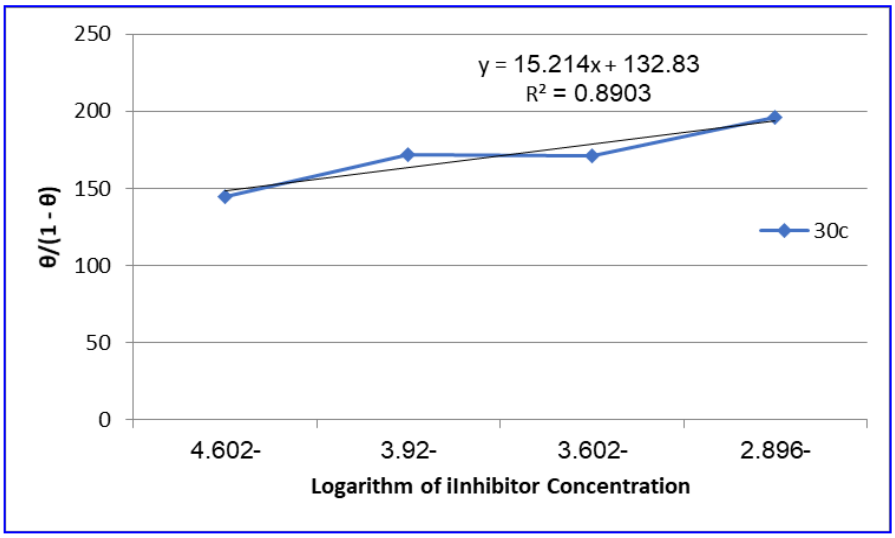


Figure (11): Temkin Adsorption Isotherm of " Fe- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 30 °C

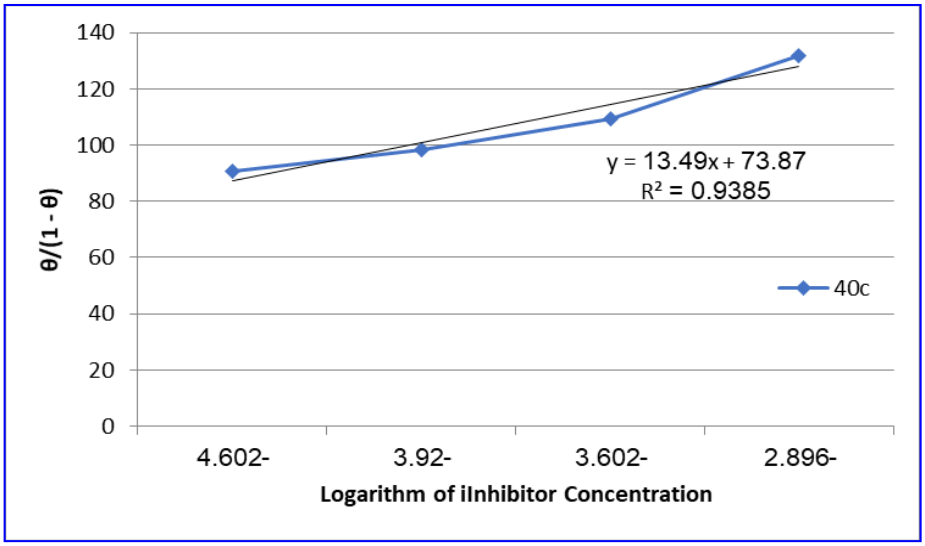


Figure (12) : Temkin Adsorption Isotherm of " Fe- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 40 °C

was found to be best fit among these four adsorption isotherms, a straight line with (R2 = 0.9606) at temperatures 30°C of Co- Chelate as shown in figure (15), as (R2) for inhibitor temperature where the value is more close to unity.

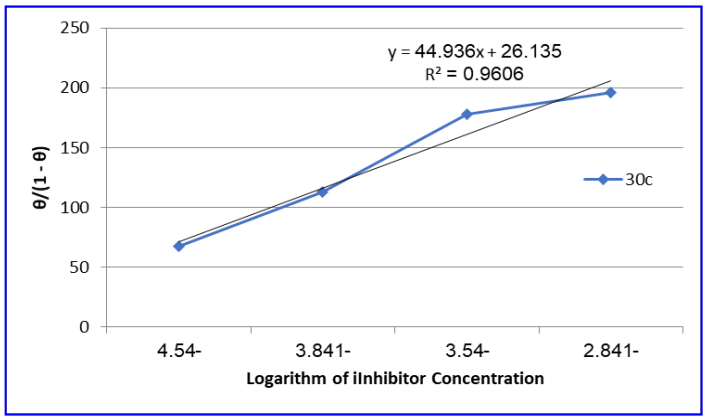


Figure (13): Temkin Adsorption Isotherm of " Co- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 30 ℃

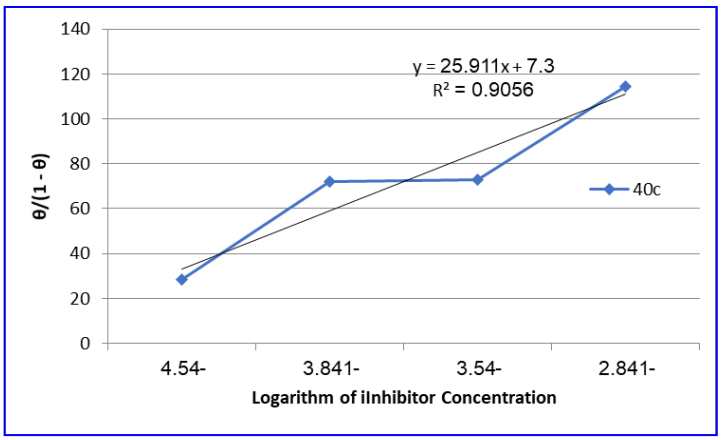


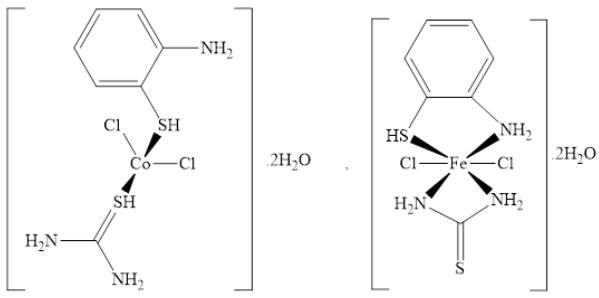
Figure (14): Temkin Adsorption Isotherm of " Co- Chelate " Inhibitor on Mild Carbon Steel in 0.5 M HCl at 40 ℃

Conclusion

Through this research, whose main objective was to study the inhibitory activity of Chelates of iron and cobalt, we present the most important results that we reached in this study on the following point:

- It was observed that the corrosion of soft steel in HCl solution decreased with increasing concentration of iron and cobalt Chelates.
- The iron and cobalt Chelates were able to reduce the corrosion rate of soft steel, and it was noted that the best result was from the cobalt solution that contains the largest concentration of the cobalt Chelate.
- With regard to the iron Chelate, as the temperature increases, the corrosion rate of soft steel increases.
- With regard to the cobalt complex, the higher the temperature, the lower the corrosion rate of soft steel.

-The general conclusion is that the corrosion resistance using Chelates is better at the lower temperature (30°C) compared to when the temperature increases at (40°C).



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may also be acknowledged.

ETHICS

Not applicable

Conflicts of Interest

The authors declare no conflicts of interest.

Author contributions: Example, A.B. developed the theoretical formalism, performed the analytic calculations and performed the numerical simulations. Both A.B and B.C. authors contributed to the final version of the manuscript. B.C. supervised the project.

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References

1. Abduljalil, N., et al., Synthesis, Characterization, Antimicrobial Activity, DFT, Molecular Docking, and ADMET of 4-Chlorophenyazolquniolin-8-ol and Its Metal Complexes. AlQalam Journal of Medical and Applied Sciences, 2024: p. 566-582.
2. Bufarwa, S.M., et al., Antituberculosis, antimicrobial, antioxidant, cytotoxicity and anti-inflammatory activity of Schiff base derived from 2, 3-diaminophenazine moiety and its metal (II) complexes: structural elucidation, computational aspects, and biological evaluation. Reviews in Inorganic Chemistry, 2025. 45(1): p. 105-124.
3. El-Ajaily, M., N. Al-Barki, and A. Maihub, Mixed schiff base chelates: synthesis ans spectroscopic investigation. Asian Journal Advanced Basic Science, 2016. 4: p. 123-130.
4. El-Ajaily, M., et al., Schiff base derived from phenylenediamine and salicylaldehyde as precursor techniques in coordination chemistry. J Chem Pharm Res, 2013. 5(12): p. 933-938.
5. Binhamad, H.A., et al., Synthesis, Characterization (IR, Elemental analysis, Molar Conductivity), and Antibacterial Investigation of Complex produced by the reaction between Co (II) ion with mixed ligands of (Amoxicillin and Salen). Al-Mukhtar J. Basic Sci, 2023. 21: p. 98-104.
6. El-Barasi, N., et al., Synthesis, characterization, theoretical study and biological evaluation of Schiff base and their La (III), Ce (IV) and UO2 (II) complexes. Bulletin of the Chemical Society of Ethiopia, 2023. 37(2): p. 335-346.
7. Mohapatra, R., et al., E-Zahan, MK (2019). Recent advances in urea-and thiourea-based metal complexes: biological, sensor, optical, and corroson inhibition studies. Comments on Inorganic Chemistry. 39(3): p. 127-187.
8. El-Ajaily, M., S. Ben-Gweirif, and A. Maihub, &El-. tajoury, AN (2005), chelation behavior and biological activity of divalent metal ions towards Schiff-base derived from salicylaldehyde and histidine. Science and it's Application Journal. 1: p. 196-210.
9. Maihub, A., et al., Synthesis of Some Mixed Ligand Complexes Derived From Catechol And 2-Aminopyridine And Their Biological Activity. Journal of basic and applied Sciences, 2005. 15(1): p. 41.
10. Bufarwa, S., et al., Synthesis, characterization, thermal, theoretical studies, antimicrobial, antioxidant activity, superoxide dismutase-like activity and catalase mimetics of metal (II) complexes derived from sugar and Schiff base. Reviews in Inorganic Chemistry, 2024. 44(4): p. 521-533.
11. Bufarwa, S., S. Abdel-Latif, and H.B. Bahnasy, Spectroscopic, Thermal, and Conductometric Studies of Some (Arylazo) Quinolin-8-Ol and Their Complexes with the Divalent Ions of Mn, Ni, Cu, and Zn. Eur. Chem. Bull, 2023. 12: p. 187-197.
12. Amin, A., et al., In silico identification of a prognostic gene signature and virtual screening for hepatocellular carcinoma. Computational Biology and Chemistry, 2025: p. 108718.
13. Hasan, H., et al., Dieckol from Brown Algae Targeting the Hepatocellular Carcinoma Pathway: A Computational Pharmacology Study. Pharmacological Research-Reports, 2025: p. 100064.
14. Bibi, S., et al., Cordycepin and its structural derivatives effectively suppress the high expression of epidermal growth factor receptor (EGFR) tyrosine kinase in breast carcinomas: a computational drug development approach. Current Medicinal Chemistry, 2025. 32(26): p. 5582-5610.
15. Mohapatra, R.K., et al., DFT, anticancer, antioxidant and molecular docking investigations of some ternary Ni (II) complexes with 2-[(E)-[4-(dimethylamino) phenyl] methyleneamino] phenol. Chemical Papers, 2021. 75(3): p. 1005-1019.
16. Ali, F., et al., Pharmacophore-Based Discovery of Licoisoflavanone as a Dual CXCR4/CXCR7 Inhibitor for Coronary Artery Disease: Integration of Traditional Chinese Medicine and Modern Computational Approaches. Journal of Computational Biophysics and Chemistry, 2025.
17. Mustapha, B., et al., Computational approach: 3D-QSAR, molecular docking, molecular dynamics simulation investigations, drug-like-ness, and DFT score evaluation of a potential novel and retrosynthesis of some TR-H derivatives as Streptococcus pneumoniae drug. Karbala International Journal of Modern Science, 2025. 11(2): p. 9.

18. Maihub, A. and M. El-Ajaily, Synthesis Characterization and Biological Applications of Schiff Base Complexes Containing Acetophenone or Resemblance Compounds. Academic Journal of Chemistry, 2018. 3(6): p. 46-59.
19. Maihub, A., M. El-Ajaily, and S. Hudere, Synthesis and spectral studies of some transition metal complexes of Schiff base. Asian Journal of Chemistry, 2007. 19(1): p. 1.
20. Bufarwa, S.M., et al. Evaluation of Some Heavy Metals (Co, Zn, Pb, and Cd) in Sardines Cans Samples Taken from Some Markets in El-Beida City-Libya. in Libyan Journal of Basic Sciences (LJBS), Special Issue for 5th International Conference for Basic Sciences and Their Applications (5th ICBSTA). 2022.
21. Morad, F., M. Elajaily, and S. Ben Gweirif, Preparation, physical characterization and antibacterial activity of Ni (II) Schiff base complex. Journal of Science and Its Applications, 2007. 1(1): p. 72-78.
22. Morad, F., M. El-Ajaily, and A. Maihub, Preparation, characterization and antibacterial activity of some metal ion complexes. Egypt J. Anal. Chem, 2006. 15: p. 98-103.
23. Maihub, A., M. El-ajaily, and N. El-Hassy, Titanium (IV), Chromium (III) and Iron (III) complexes of Schiff base derived from aldehyde and primary amine. International Journal of ChemTech Research, 2012. 4: p. 631-633.
24. Saleh, M., et al., Algal Bioremediation: Heavy Metals Removal And Evaluation Of Biological Activities In Sewage Plant. Journal of Survey in Fisheries Sciences, 2023: p. 1355-65.
25. Saeed, S., et al., Utilizing Microbiological Techniques: The Residual Microorganisms in Poultry Flesh Raised at Random Between 2024 and 2025. AlQalam Journal of Medical and Applied Sciences, 2025: p. 958-960.
26. Abbass, L.M., et al., Exploring the anti-colon cancer potential of febuxostat-based mixed metal complexes with 2, 2′ -bipyridine: MTT assay, toxicity evaluation, prediction profiles, and computational studies. Inorganic Chemistry Communications, 2025. 178: p. 114460.
27. Hamil, A., et al., Synthesis of a New Schiff Base: 2-[2-(E)-(2-hydroxyphenyl)-ethylidene] aminoethyl) ethanimidoyl] phen. International Journal of ChemTech Research, 2012. 4(2): p. 682-685.
28. Mohapatra, R.K., et al., biological aspects of Schiff base–metal complexes derived from benzaldehydes: an overview. Journal of the Iranian Chemical Society, 2018. 15(10): p. 2193-2227.
29. Mohapatra, R.K., et al., Synthesis, spectral, thermal, kinetic and antibacterial studies of transition metal complexes with benzimidazolyl-2-hydrazones of o-hydroxyacetophenone, o-hydroxybenzophenone and o-vanillin. Bulletin of the Chemical Society of Ethiopia, 2018. 32(3): p. 437-450.
30. El-ajaily, M., et al., Experimental studies of azo Schiff base chelates and their corrosion inhibition behavior. Asian J. Adv. Basic Sci, 2014. 2(2): p. 17-30.
31. El-Ajaily, M., et al., Mixed-Ligand Chelate Formation of Co (II), Ni (II), Cu (II) and Zn (II) Ions with Schiff Base as Main Ligand and Amino Acid as Co-Ligand. International Research Journal of Pure and Applied Chemistry, 2015. 5(3): p. 229.
32. Hamil, A.M. and M.M. El-Ajaily, Synthesis and Physiochemical Investigation of Cobalt (II) and Nickel (II) Complexes of 1-2-[(Z)-2-(3-acetyl-4-hydroxyphenyl)-1-diazenyl] phenyl-1-ethanone. Journal of the Chemical Society of Pakistan, 2011. 33(6): p. 652.
33. Elajaily, M.M., et al., Synthesis, characterization and corrosion inhibition of cobalt (II) azo schiff base chelate. J Chem Pharm Res, 2013. 5(12): p. 1144-1151.
34. El-Ajaily, M., et al., Complex Formation of TiO (IV), Cr (III) and Pb (II) ions Using 1, 3-bis (2-hydroxybenzylidene) Thiourea as Ligand. Egyptian Journal of Analytical Chemistry, 2011. 20(16): p. 18-25.
35. Al-Resayes, S.I., et al., Synthesis, characterization, biological applications, and molecular docking studies of amino-phenol-derived mixed-ligand complexes with Fe (III), Cr (III), and La (III) ions. Journal of Saudi Chemical Society, 2023. 27(3).
36. Miloud, M., et al., Antifungal activity of some mixed ligand complexes incorporating Schiff bases. J Bacteriol Mycol, 2020. 7(1): p. 1122.
37. El-Barasi, N.M., et al., Synthesis, structural investigations and antimicrobial studies of hydrazone based ternary complexes with Cr (III), Fe (III) and La (III) ions. Journal of Saudi Chemical Society, 2020. 24(6): p. 492-503.
38. Mustapha, B., Synthèse et caractérisation de complexes de Zn (II), Hg (II) et Pb (II) avec quelques dérivés du 1, 2, 3-Triazole. 2007.
39. El-ajaily, M.M., et al., Transition Metal Complexes of (E)-2 ((2-hydroxybenzylidene) amino-3-mercaptopropanoic acid: XRD, Anticancer, Molecular modeling and Molecular Docking Studies. ChemistrySelect, 2019. 4(34): p. 9999-10005.
40. Bufarwa, S. and S. Abdel-Latif, Spectroscopic, thermal, and conductometric investigation of some (arylazo) quinolin-8-ol and their complexes with the divalent ions of Mn, Ni, Cu, and Zn. 2022.
41. BELAIDI, M., et al., Integrated 3D-QSAR, Molecular Docking, Molecular Dynamics Simulation, ADMET, Drug-Likeness, and DFT Score Evaluation of a Potential Novel 1, 2, 3-Triazole-Hybrid Streptococcus Pneumoniae Drug. Molecular Docking, Molecular Dynamics Simulation, ADMET, Drug-Likeness, and DFT Score Evaluation of a Potential Novel. 1(2).

42. Mustapha, B., et al., Exploring the Antituberculosis, Anti-Inflammatory, and Antimicrobial Activities and Computational Potential of Quinoline-8-ol Azo Dye Complexes. Applied Organometallic Chemistry, 2025. 39(8): p. e70310.
43. Abdullah, F. I., Elajaily, M. M., Suliman, R. O. M., & Maihub, A. A. (2014). Preparation, Spectroscopic investigation and Corrosion inhibition of some azo Schiff base chelates. Int. J. Adv. Pharm. Biol. Chem., 3(2), 256-265.
44. El-ajaily, M. M., Abdullah, F. I., Suliman, M. S., & Akasha, R. A. (2014). Experimental studies of azo Schiff base chelates and their corrosion inhibition behavior. Asian J. Adv. Basic Sci, 2(2), 17-30.
45. Elajaily, M. M., Abdullah, F. I., Akasha, R. A., & Suliman, M. S. (2013). Synthesis, characterization and corrosion inhibition of cobalt (II) azo schiff base chelate. J Chem Pharm Res, 5(12), 1144-1151.
46. Saber, Y., Ibrahim, N., & Bufarwa, S. (2025). Pharmacological and Computational Assessment of Co (II), Cu (II), Ni (II), and Zn (II) Schiff Base Complexes: Anticancer, Antioxidant, and Antibacterial Investigations. AlManar Journal of Medical and Applied Sciences, 1(1), 20-33.
47. A. Abdu Al-Zahra Rashq Al-sadi, Study of Polarization Curves for the Carbon Steel (X65-Steel) in Acidic Media memoir de Master, Al-Qadisiya University, Iraq, (2016).
48. H. Shahbeig, N. Bagheri, S. A. Ghorbanian, A. Hallajisani, and S. Poorkarimi, “A new adsorption isotherm model of aqueous solutions on granular activated carbon,” World J. Model. Simul., vol. 9, no. 4, pp. 243–254, (2013).
49. 16. M. Suliman, M. Alkilani, T. Abdullah, M. Ali, The Effect of Methyle Carbazodithoate" Corrosion inhibitor on Corrosion Behaviour of Low Carbon Steels in Acid Solution at Different Temperatures, Journal of Pure & Applied Sciences Vol.18 No. 4 (2019).